

Adiabatic geometric phases in hydrogenlike atoms

Erik Sjöqvist^{1*}, X. X. Yi^{2†}, and Johan Åberg^{1‡}

¹*Department of Quantum Chemistry, Uppsala University, Box 518, Se-751 20 Uppsala, Sweden*

²*Department of Physics, Dalian University of Technology, Dalian 116024, China*

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We examine the effect of spin-orbit coupling on geometric phases in hydrogenlike atoms exposed to a slowly varying magnetic field. The marginal geometric phases associated with the orbital angular momentum and the intrinsic spin fulfill a sum rule that explicitly relates them to the corresponding geometric phase of the whole system. The marginal geometric phases in the Zeeman and Paschen-Back limit are analyzed. We point out the existence of nodal points in the marginal phases that may be detected by topological means.

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Imagine a quantal spin evolving under influence of a magnetic field so that the initial and final states of the spin coincide. Cyclic evolution of this kind results in a phase factor divisible into a dynamic part and a part that only depends upon the global geometry associated with the evolution of the spin. The latter is the geometric phase, first delineated by Berry [1] in the adiabatic case. This adiabatic geometric phase is proportional to the solid angle enclosed by the direction of a slowly changing magnetic field and where the proportionality factor is given by the spin projection quantum number. The geometric phase structure for this system resembles exactly that of a charged particle in a magnetic monopole field. A similar result in the special case of spin- $\frac{1}{2}$ was subsequently found for nonadiabatic evolution [2], in case of which the solid angle is the area enclosed on the Bloch sphere.

These results opened up the possibility to study magnetic monopole structures in the laboratory; a fact that has triggered considerable interest in the geometric phase for quantal systems carrying angular momentum. Extensions of the spin-monopole problem to systems consisting of several coupled angular momenta have been theoretically put forward [3, 4, 5, 6, 7, 8, 9] and experimentally implemented [10, 11]. In particular, the issue concerning the relation between the overall geometric phase and the geometric phases of the subsystems has been addressed for adiabatically evolving pairs of uniaxially coupled spin- $\frac{1}{2}$ [12, 13].

Coupling generally leads to entangled multiparticle systems, which implies that the marginal states of the concomitant subsystems are mixed. Geometric phases for mixed states take the form of weighted averages of geometric phase factors, with weight factors given by the time-independent [14] or time-dependent [15] eigenvalues of the corresponding marginal states.

In this paper, we address the issue of coupled angular

momenta in terms of hydrogenlike atoms coupled to a slowly varying magnetic field. For such systems, there is a natural bipartite decomposition of the total angular momentum into two subsystems consisting of the orbital part (L) and the intrinsic spin part (S), exposed to spin-orbit (LS) coupling. We wish to examine the effect of the LS coupling on the overall geometric phase as well as on those pertaining to the two subsystems.

Consider a hydrogenlike atom driven by a uniform magnetic field $\mathbf{B} = B_0 \mathbf{n}$ with B_0 the nonzero magnetic field strength and $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, θ and ϕ being slowly varying parameters. Let \mathbf{L} and \mathbf{S} be the orbital angular momentum and intrinsic spin, respectively. The spin-orbit Hamiltonian reads [16]

$$\begin{aligned} H_{\mathbf{n}} &= g\mathbf{n} \cdot (\mathbf{L} + 2\mathbf{S}) + 2\mathbf{L} \cdot \mathbf{S} \\ &= U_L(\theta, \phi) U_S(\theta, \phi) H_z U_L^\dagger(\theta, \phi) U_S^\dagger(\theta, \phi) \\ &= U_J(\theta, \phi) H_z U_J^\dagger(\theta, \phi), \end{aligned} \quad (1)$$

where we may choose ($\hbar = 1$ from now on)

$$U_X(\theta, \phi) = e^{-i\phi X_z} e^{-i\theta X_y} e^{i\phi X_z}, \quad X = L, S, J, \quad (2)$$

$\mathbf{J} = \mathbf{L} + \mathbf{S}$ being the total angular momentum. Here, g is the Zeeman-LS strength ratio, H_z is the Hamiltonian at the north pole $\mathbf{n} = (0, 0, 1)$ of the parameter sphere, and $[H_z, J_z] = 0$; the latter implying that the eigenvectors of H_z can be labeled by the eigenvalues μ of J_z .

H_z is block-diagonalizable in one- and two-dimensional blocks with respect to the product basis with elements $|l, m\rangle|\frac{1}{2}, \pm\frac{1}{2}\rangle \equiv |l, m\rangle|\pm\rangle$ being the common eigenvectors of $\mathbf{L}^2, L_z, \mathbf{S}^2, S_z$. Each block may be labeled by the eigenvalue $\mu = -l - \frac{1}{2}, -l + \frac{1}{2}, \dots, l + \frac{1}{2}$ of J_z . The two extremal subspaces characterized by $|\mu| = l + \frac{1}{2} \equiv \mu_e$ are one-dimensional corresponding to the two product vectors

$$|\psi^{(l; \pm\mu_e)}\rangle = |l, \pm l\rangle|\pm\rangle. \quad (3)$$

The remaining blocks are two-dimensional, each of which corresponding to the vectors $|l, m = \mu - \frac{1}{2}\rangle|+\rangle, |l, m + 1 = \mu + \frac{1}{2}\rangle|-\rangle$, $|\mu| < l + \frac{1}{2}$. For each such μ , the corresponding

*Electronic address: eriks@kvac.uu.se

†Electronic address: yixx@dlut.edu.cn

‡Electronic address: johan.berg@kvac.uu.se

two-dimensional Hamiltonian suboperator has the form

$$H_z^{(l;\mu)} = E^{(l;\mu)} I^{(l;\mu)} + \Delta E^{(l;\mu)} \left(\sin \alpha^{(l;\mu)} \sigma_x^{(l;\mu)} + \cos \alpha^{(l;\mu)} \sigma_z^{(l;\mu)} \right), \quad (4)$$

with $I^{(l;\mu)}$, $\sigma_x^{(l;\mu)}$, and $\sigma_z^{(l;\mu)}$ the standard unit and Pauli operators acting on the relevant subspace. Furthermore

$$\begin{aligned} E^{(l;\mu)} &= g\mu - \frac{1}{2}, \\ \Delta E^{(l;\mu)} &= \frac{1}{2} \sqrt{g^2 + 4g\mu + (2l+1)^2}, \\ \cos \alpha^{(l;\mu)} &= \frac{2\mu + g}{\sqrt{g^2 + 4g\mu + (2l+1)^2}}, \end{aligned} \quad (5)$$

in terms of which the energy eigenvalues read $E_{\pm}^{(l;\mu)} = E^{(l;\mu)} \pm \Delta E^{(l;\mu)}$ with corresponding entangled eigenvectors

$$\begin{aligned} |\psi_+^{(l;\mu)}\rangle &= \cos\left(\frac{1}{2}\alpha^{(l;\mu)}\right) |l, \mu - \frac{1}{2}\rangle|+\rangle \\ &\quad + \sin\left(\frac{1}{2}\alpha^{(l;\mu)}\right) |l, \mu + \frac{1}{2}\rangle|-\rangle, \\ |\psi_-^{(l;\mu)}\rangle &= -\sin\left(\frac{1}{2}\alpha^{(l;\mu)}\right) |l, \mu - \frac{1}{2}\rangle|+\rangle \\ &\quad + \cos\left(\frac{1}{2}\alpha^{(l;\mu)}\right) |l, \mu + \frac{1}{2}\rangle|-\rangle. \end{aligned} \quad (6)$$

The g -dependence of the eigenvectors is due to the fact that the Zeeman and LS term do not commute.

With the above choice of rotation operators, we have $U_X(0, \phi) = I$ and $U_X(\pi, \phi) = e^{-i\pi X_y} e^{2i\phi X_z}$. This entails that the corresponding energy eigenvectors cannot be unique simultaneously at the north and south pole. For example, by choosing the phase of the eigenvectors $|\psi^{(l;\mu)}\rangle$ of H_z to be independent of ϕ , as in Eqs. (3) and (6), the resulting instantaneous eigenvectors $U_X(\theta, \phi)|\psi^{(l;\mu)}\rangle$ are unique at the north pole but yields a singular gauge potential at the south pole. For the same reference eigenvectors, one may move this singularity to the north pole by instead choosing the rotation operators $\tilde{U}_X(\theta, \phi) = e^{-i\phi X_z} e^{-i\theta X_y} e^{-i\phi X_z}$. On the other hand, the section [17] $\{U_X(\theta, \phi), \theta \in [0, \pi]; \tilde{U}_X(\theta, \phi), \theta \in (0, \pi]\}$ is globally well-defined for any choice of eigenvectors of H_z . This single-valued section captures the monopole structure corresponding to the $2j+1$ fold degeneracy at $g=0$, j being the eigenvalue of \mathbf{J}^2 .

We now compute the adiabatic geometric phases for the atom and its subsystems L and S under the assumption $g \neq 0$. Let us start with the extremal states $\mu = \pm\mu_e$. We note that

$$|\psi^{(l;\pm\mu_e)}; \theta, \phi\rangle = U_L(\theta, \phi)|l, \pm l\rangle U_S(\theta, \phi)|\pm\rangle \quad (7)$$

are product eigenvectors of $H_{\mathbf{n}}$. Assume that the external magnetic field slowly traverses a loop \mathcal{C} such that the adiabatic approximation is valid. Then, the adiabatic geometric phase becomes

$$\Gamma_J^{(l;\pm\mu_e)}[\mathcal{C}] = \mp\mu_e\Omega \quad (8)$$

with Ω the solid angle enclosed by the loop. From the product form of the extremal states, we obtain the corresponding marginal geometric phases for L and S as $\mp l\Omega$ and $\mp \frac{1}{2}\Omega$, respectively, which are g -independent and sum up to $\Gamma_J^{(l;\pm\mu_e)}[\mathcal{C}]$ since $\mu_e = l + \frac{1}{2}$.

Next we compute the adiabatic geometric phases for $|\mu| < l + \frac{1}{2}$. The eigenvectors of the instantaneous Hamiltonian $H_{\mathbf{n}}$ take the form

$$\begin{aligned} |\psi_{\pm}^{(l;\mu)}; \theta, \phi\rangle &= U_J(\theta, \phi)|\psi_{\pm}^{(l;\mu)}\rangle \\ &= U_L(\theta, \phi)U_S(\theta, \phi)|\psi_{\pm}^{(l;\mu)}\rangle. \end{aligned} \quad (9)$$

We obtain the g -independent pure state geometric phase as

$$\Gamma_{J,\pm}^{(l;\mu)}[\mathcal{C}] = -\mu\Omega, \quad (10)$$

which follows directly from the fact that the energy eigenvectors $|\psi_{\pm}^{(l;\mu)}; \theta, \phi\rangle$ are also eigenvectors of $\mathbf{n} \cdot \mathbf{J}$ both with the eigenvalue μ . The marginal states read

$$\begin{aligned} \rho_{L,\pm}^{(l;\mu)}(\theta, \phi) &= \text{Tr}_S |\psi_{\pm}^{(l;\mu)}; \theta, \phi\rangle \langle \psi_{\pm}^{(l;\mu)}; \theta, \phi| \\ &= U_L(\theta, \phi) \rho_{L,\pm}^{(l;\mu)} U_L^\dagger(\theta, \phi), \\ \rho_{S,\pm}^{(l;\mu)}(\theta, \phi) &= \text{Tr}_L |\psi_{\pm}^{(l;\mu)}; \theta, \phi\rangle \langle \psi_{\pm}^{(l;\mu)}; \theta, \phi| \\ &= U_S(\theta, \phi) \rho_{S,\pm}^{(l;\mu)} U_S^\dagger(\theta, \phi), \end{aligned} \quad (11)$$

with

$$\begin{aligned} \rho_{L,\pm}^{(l;\mu)} &= \text{Tr}_S |\psi_{\pm}^{(l;\mu)}\rangle \langle \psi_{\pm}^{(l;\mu)}| \\ &= \frac{1}{2} \left(1 \pm \cos \alpha^{(l;\mu)} \right) |l, \mu - \frac{1}{2}\rangle \langle l, \mu - \frac{1}{2}| \\ &\quad + \frac{1}{2} \left(1 \mp \cos \alpha^{(l;\mu)} \right) |l, \mu + \frac{1}{2}\rangle \langle l, \mu + \frac{1}{2}|, \\ \rho_{S,\pm}^{(l;\mu)} &= \text{Tr}_L |\psi_{\pm}^{(l;\mu)}\rangle \langle \psi_{\pm}^{(l;\mu)}| \\ &= \frac{1}{2} \left(1 \pm \cos \alpha^{(l;\mu)} \right) |+\rangle \langle +| \\ &\quad + \frac{1}{2} \left(1 \mp \cos \alpha^{(l;\mu)} \right) |-\rangle \langle -|. \end{aligned} \quad (12)$$

Since the marginal density operators $\rho_{L,\pm}^{(l;\mu)}$ and $\rho_{S,\pm}^{(l;\mu)}$ evolve unitarily under U_L and U_S , respectively, it follows that the marginal geometric phases can be computed using the approach in Ref. [14]. Explicitly, for a magnetic field whose direction traces out a loop \mathcal{C} , this yields

$$\begin{aligned}
\exp\left(i\Gamma_{L,\pm}^{(l;\mu)}[\mathcal{C};g]\right) &= \Phi\left[\left(1 \pm \cos\alpha^{(l;\mu)}\right)e^{-i(\mu-\frac{1}{2})\Omega} + \left(1 \mp \cos\alpha^{(l;\mu)}\right)e^{-i(\mu+\frac{1}{2})\Omega}\right] \\
&\Rightarrow \Gamma_{L,\pm}^{(l;\mu)}[\mathcal{C};g] = -\mu\Omega \pm \arctan\left(\cos\alpha^{(l;\mu)}\tan\frac{\Omega}{2}\right), \\
\exp\left(i\Gamma_{S,\pm}^{(l;\mu)}[\mathcal{C};g]\right) &= \Phi\left[\left(1 \pm \cos\alpha^{(l;\mu)}\right)e^{-i\Omega/2} + \left(1 \mp \cos\alpha^{(l;\mu)}\right)e^{i\Omega/2}\right] \\
&\Rightarrow \Gamma_{S,\pm}^{(l;\mu)}[\mathcal{C};g] = \mp \arctan\left(\cos\alpha^{(l;\mu)}\tan\frac{\Omega}{2}\right). \tag{13}
\end{aligned}$$

Here, $\Phi[z] = z/|z|$ for any nonzero complex number z . Notice that the above marginal geometric phases are g -dependent through $\cos\alpha^{(l;\mu)}$. They obey the symmetry $\Gamma_{X,\pm}^{(l;\mu)}[\mathcal{C};-g] = -\Gamma_{X,\pm}^{(l;\mu)}[\mathcal{C};g]$, $X = L, S$, which is expected since the change $(\mu, g, \Omega) \rightarrow (-\mu, -g, \Omega)$ is physically equivalent to reversing the orientation of the loop \mathcal{C} . Furthermore, by comparing Eqs. (10) and (13), it follows that the marginal geometric phases of the L and S subsystems fulfill the sum rule

$$\Gamma_{L,\pm}^{(l;\mu)}[\mathcal{C};g] + \Gamma_{S,\pm}^{(l;\mu)}[\mathcal{C};g] = \Gamma_{J,\pm}^{(l;\mu)}[\mathcal{C}] \tag{14}$$

that explicitly relates them to the corresponding geometric phases for the pure entangled states.

Let us now consider the extreme cases $|g| \gg 1$ (Paschen-Back regime [18]) and $0 < |g| \ll 1$ (Zeeman regime). In the Paschen-Back limit, we have $\cos\alpha^{(l;\mu)} \approx 1$, which implies

$$\begin{aligned}
\Gamma_{S,\pm}^{(l;\mu)}[\mathcal{C};g] &\approx \mp \frac{1}{2}\Omega, \\
\Gamma_{L,\pm}^{(l;\mu)}[\mathcal{C};g] &\approx -\left(\mu \mp \frac{1}{2}\right)\Omega. \tag{15}
\end{aligned}$$

These phases are those of the pure vectors $U_S(\theta, \phi)|\pm\rangle$ and $U_L(\theta, \phi)|l, \mu \pm \frac{1}{2}\rangle$, respectively, as expected as the LS term in $H_{\mathbf{n}}$ is negligible in this limit. The Zeeman condition $0 < |g| \ll 1$ yields $\cos\alpha^{(l;\mu)} \approx \mu/(l+\frac{1}{2})$, leading to

$$\begin{aligned}
\Gamma_{S,\pm}^{(l;\mu)}[\mathcal{C};g] &\approx \mp \arctan\left(\frac{\mu}{l+\frac{1}{2}}\tan\frac{\Omega}{2}\right), \\
\Gamma_{L,\pm}^{(l;\mu)}[\mathcal{C};g] &\approx -\mu\Omega \pm \arctan\left(\frac{\mu}{l+\frac{1}{2}}\tan\frac{\Omega}{2}\right). \tag{16}
\end{aligned}$$

From this we can conclude that the marginal geometric phases may in general not be small for $0 < g \ll 1$, contrary to the cases discussed in Refs. [12, 13], where all geometric phases were found to be quenched in this regime due to the uniaxial coupling term. The reason for this quenching effect in the uniaxial case is that the coupling term defines a fixed preferred quantization axis that makes the eigenstates essentially unaffected by a weak magnetic field. In the LS case, though, no particular direction in space is singled out by the spherically symmetric coupling term and the quantization axis of

the instantaneous eigenstates still coincides with the direction of the applied magnetic field. This feature is true no matter how small g is as long as it is nonzero. On the other hand, if $g = 0$, then the magnetic field decouples from the atom and no change in the atomic eigenstates can take place when the direction of the magnetic field varies. Thus, $g = 0$ is a singular point in the sense that the geometric phases become independent of the enclosed solid angle Ω of the magnetic field. It should be noted that the same singular behavior is present for the standard case [1] of a single spin in a slowly rotating magnetic field. In physically realistic scenarios, though, it is reasonable to expect that the singularity at $g = 0$ becomes invisible as the atom is increasingly exposed to noise and decoherence effects.

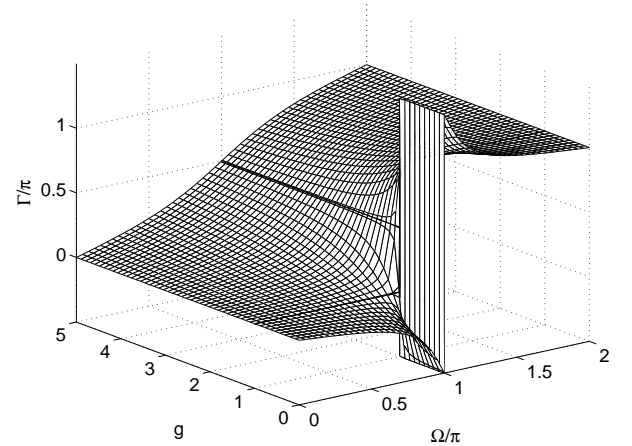


FIG. 1: Adiabatic geometric phase $\Gamma_{S,-}^{(2;-1/2)}[\mathcal{C};g]$ of the intrinsic spin as a function of the dimensionless Zeeman-LS coupling strength ratio g and solid angle Ω enclosed by the loop \mathcal{C} of the magnetic field.

The geometric phase $\Gamma_{S,-}^{(2;-1/2)}[\mathcal{C};g]$ of the intrinsic spin as a function of coupling strength g and solid angle Ω is shown in Fig. 1. Notice in particular that this graph confirms the expected asymptotic behavior in the Paschen-Back limit $|g| \gg 1$.

The marginal density operators are degenerate when $\cos\alpha^{(l;\mu)} = 0$, which happens along the line $g = -2\mu$

in the space spanned by (Ω, g) . For $\mu = -\frac{1}{2}$ this line occurs at $g = 1$, as indicated in Fig. 1. While the cyclic geometric phase of the whole system is well-defined at these lines, the corresponding marginal geometric phases are undefined there [14]. Furthermore, the visibilities of the subsystems, defined as [14]

$$\begin{aligned} \mathcal{V}_{\pm, S}^{(l; \mu)}[\mathcal{C}; g] &= \mathcal{V}_{\pm, L}^{(l; \mu)}[\mathcal{C}; g] \\ &\equiv \frac{1}{2} \left| \left(1 \pm \cos \alpha^{(l; \mu)} \right) e^{-i\Omega/2} \right. \\ &\quad \left. + \left(1 \mp \cos \alpha^{(l; \mu)} \right) e^{i\Omega/2} \right|, \end{aligned} \quad (17)$$

reduces to

$$\mathcal{V}_{\pm, S}^{(l; \mu)}[\mathcal{C}; g] = \mathcal{V}_{\pm, L}^{(l; \mu)}[\mathcal{C}; g] = \left| \cos \frac{\Omega}{2} \right| \quad (18)$$

at the points where the marginal geometric phases are undefined. The marginal visibilities vanish at their common nodal points $\Omega = (2p + 1)\pi$, p integer, which is manifested as a jump at $(\Omega, g) = (\pi, 1)$ in Fig. 1. These nodal points can be detected topologically by considering loops in the space spanned by (Ω, g) . By continuously monitoring the marginal phases along a loop, a resulting

2π phase shift signals the existence of such a nodal point [19]. For example, as indicated in Fig. 1, by traversing a loop in the counterclockwise (clockwise) direction such that it encloses the singular point at $(\Omega, g) = (\pi, 1)$ once, we end up at a phase shift 2π (-2π).

In conclusion, we have computed adiabatic geometric phases in hydrogenlike atoms coupled to a slowly varying magnetic field. We have shown that while the total geometric phase is independent of the strength of the spin-orbit coupling, this is not the case for the corresponding marginal phases. It turns out, though, that the latter phases sum up to the pure state geometric phase of the whole system. Further consideration as to the generality of this sum rule for other systems of coupled angular momenta seems pertinent. We have examined the marginal geometric phases in the Zeeman and Paschen-Back limit. Finally, we have pointed out the existence of nodal points where the marginal geometric phases become undefined and we have argued that these points may be detected by topological means.

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